

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 335 °C

Global applicability domain: Outside

Local applicability domain index: 1.95e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Sulfonmethane</div> <div>Measured: 300</div> <div>Predicted: 295</div>	<div>Image not found</div> <div>Parathion</div> <div>Measured: 375</div> <div>Predicted: 362</div>	<div>Image not found</div> <div>Benzene, 1,1'-sulfonylbis[4-methyl-</div> <div>Measured: 406</div> <div>Predicted: 360</div>
<div>Image not found</div> <div>(+/-)-Oxychlordane</div> <div>Measured: 353</div> <div>Predicted: 346</div>	<div>Image not found</div> <div>Phenyl phosphorodichloridate</div> <div>Measured: 242</div> <div>Predicted: 255</div>	